APPENDIX F

GROUNDWATER MODELING

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APPENDIX F
GROUNDWATER MODELING

As part of the TP RI/FS, a three-dimensional groundwater flow and contaminant transport modeling analysis was performed. The analysis included the development and use of a groundwater flow model and a companion particle tracking model. The role of the flow and particle tracking model in this RI/FS was to assist in formulating appropriate questions concerning the remedial planning and design problems for the site, and to help obtain quantitative answers of sufficient accuracy and detail to guide in the decision-making process for remedial action at the site.

The model developed in this groundwater analysis performs three valuable functions:

- Organization - One of the major problems encountered in planning or design is to represent and display in simple terms the numerous characteristics of complex systems. Models provide a basis for such representation and for actually carrying out much of the computation which is required for this organization.

- Amplification - When properly used, models can amplify available knowledge of the behavior of complex systems. Models do not produce new information; however, they permit the extraction of greater amounts of information from the existing data base. In this sense they increase understanding of the problem and of the possible solutions.

- Evaluation - Models can be designed to incorporate measures of performance of the system in them, and to produce comparative evaluations of performance. Modeling can help project or predict the consequences of alternative future actions, including the no action alternative.

Models represent the behavior and performance of the complex real world aquifer system and therefore can be very powerful analytical tools, depending on the skill of application. It should be remembered, however, that they are an approximation of the real world system and not completely equivalent to it in all respects.

The major goals of this groundwater modeling analysis were to adequately characterize the potential extent of contamination through model simulation, and to predict future attenuation and migration patterns under various remedial action alternatives. Details of model development and application are described in the following sections.

F.1 GROUNDWATER FLOW MODEL DEVELOPMENT

The first step in any groundwater flow or contaminant transport study is to develop a hydraulic or flow model for the aquifer system. A groundwater flow model provides the means for evaluating the stress and effect relationships of groundwater flow. The flow model alos provides the groundwater velocity field for a companion contaminant transport model. For simple cases where only gross estimations are desired, the flow model can be as basic as a uniform flow field. For moderately complex cases where groundwater flow is essentially two-dimensional, a two-dimensional numerical computer model may be more appropriate. For more complex cases where groundwater flow must be represented in three dimensions, as is the case for the TP Site, a three-dimensional numerical computer model is necessary.

Digital computer models are capable of solving the large set of simultaneous equations that are involved in studying cause and effect relationships in heterogeneous aquifer systems with a wide variety of boundary conditions. The variable lithology (sand, silt, clay, fractured bedrock, etc.) and the complex recharge/discharge boundary system (streams and rainfall) at the TP Site require an analysis procedure beyond ordinary analytical methods. A valid digital computer model can be used to predict the effects of variations in pumpage and climatic conditions on aquifer system water levels. Head changes predicted by the model can then be used to analyze directions and extent of contaminant movement.

F.1.1 MODEL DESCRIPTION

The groundwater flow model code used in this analysis is the DYNFLOW (DYNamic groundwater FLOW simulation) computer program developed by Camp Dresser & McKee Inc. (CDM) in 1984. This code uses a Galerkin finite element formulation to solve the partial differential equation that describes the transient, three-dimensional flow of a homogeneous incompressible fluid through a heterogeneous, anisotropic medium. The program uses linear finite elements and incorporates induced infiltration from streams, artificial and natural recharge or discharge, and heterogeneous and anisotropic hydraulic properties. The program handles both linear (confined) and nonlinear (unconfined) aquifer flow conditions, and has special routines to handle a change in status from a confined to an unconfined situation. The program also has a "rising water" scheme to allow drainage to local streams, if the potential head in a phreatic aquifer rises to the elevation of the stream bed or land surface.

Numerical Method

The governing equation for three-dimensional groundwater flow is as follows:

$$S_s \frac{Mh}{Mt} = \frac{M}{Mx}\left(K_x \frac{Mh}{Mx}\right) + \frac{M}{My}\left(K_y \frac{Mh}{My}\right) + \frac{M}{Mz}\left(K_z \frac{Mh}{Mz}\right)$$

where,

h	=	hydraulic head (length)
K_x,K_y,K_z	=	principal components of the hydraulic conductivity tensor (x, y, and z assumed to be the principal directions) (length/time)
S_s	=	specific storativity (1/length)
t	=	time

This equation is based on two laws of groundwater flow. The first is Darcy's Law, which states that flow "Q" in any direction is directly proportional to the head gradient "dh/ds" in that direction. The second is the Law of Mass Conservation, which requires that the net flow from a volume of aquifer equal the rate of change of storage in that volume.

Exact mathematical solutions to this partial differential equation of flow under complex boundary and initial conditions are not known, but numerical solutions of high accuracy can be obtained using a digital computer. As stated previously, DYNFLOW uses a Galerkin finite element technique to solve this equation. In concept, the finite element method involves the following steps:

- Divide the region under consideration into a finite number of discrete sub-regions (elements) with simple geometries. In DYNFLOW, the basic working element in three dimensions is a vertical triangular prism with six nodes as shown in **Figure F-1**.

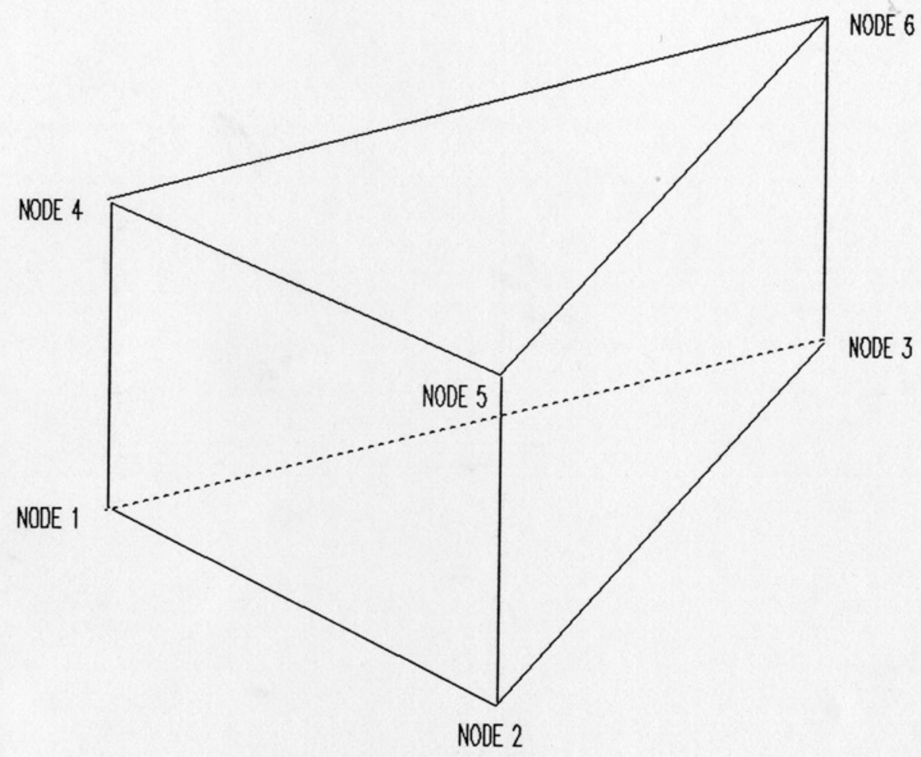
- Assume the manner in which the hydraulic head, h, can vary throughout each element (i.e., linear variation, quadratic variation, etc.). In DYNFLOW, the head varies linearly throughout the element.

- On the basis of the simple element geometry and the assumption of the hydraulic potential variation, write (local) equations for flux in terms of the hydraulic head at selected points (nodes) on the boundary of each element.

- Assemble the equations for each element (local) into a regional (global) system of equations.

- Solve the regional (global) system of equations for the hydraulic head or flux at each node. In DYNFLOW, the equations are solved by Gaussian Elimination.

The application of the finite element method as used by DYNFLOW is documented in the DYNFLOW Users Manual (CDM, 1984a). In addition, several excellent descriptions of the Galerkin technique exist in the literature (Wilson et al., 1979; Pinder and Gray, 1977).



THREE–DIMENSIONAL WORKING ELEMENT

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

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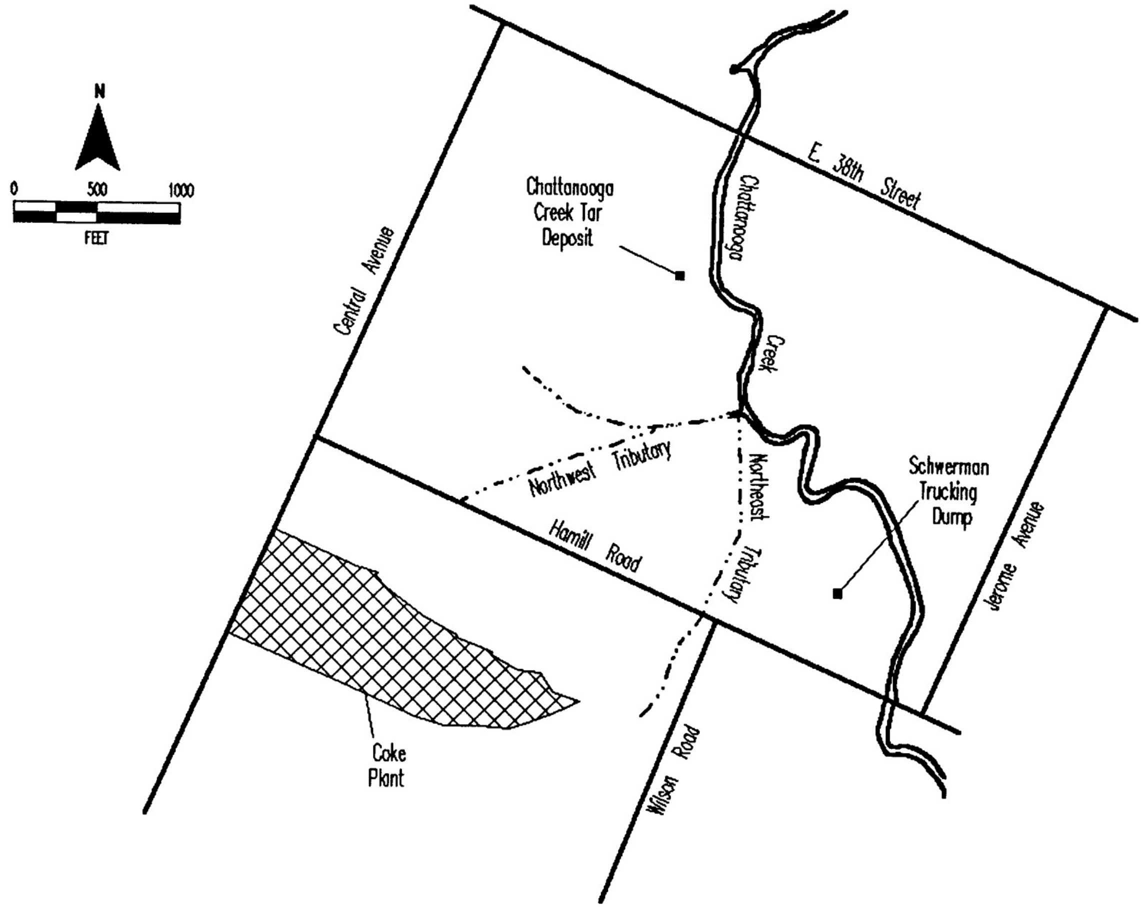
<u>Data Requirements</u>

The first step in applying this model to a specific area is to develop the finite element grid system. The X, Y, and Z coordinates for each node must be input into the model. Generally, the X and Y coordinates are user-dependent (specified by the user) and are chosen to represent significant hydrogeologic features. The Z coordinate is usually chosen to represent the top of some hydrostratigraphic unit.

The second step in the application of this model is the specification of hydrogeologic properties for each element. The hydrogeologic properties include both horizontal and vertical hydraulic conductivity, and the specific storativity or specific yield of the unit if transient (changing with time) simulations are to be performed. Other hydrogeologic conditions, including boundary conditions, rainfall recharge, starting head elevations, and well pumpages, must also be specified where appropriate.

F.1.2 FLOW MODEL SETUP

The numerical computer model described above provides the mechanism for simulating aquifer water levels. The impacts of rainfall and surface water recharge/discharge are provided by analysis of the model results. Once groundwater levels are produced, contaminant movement may be determined. This section describes how the groundwater flow model was developed for the TP Site. The base map used in the groundwater modeling analysis is shown in **Figure F-2**



SITE BASE MAP

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

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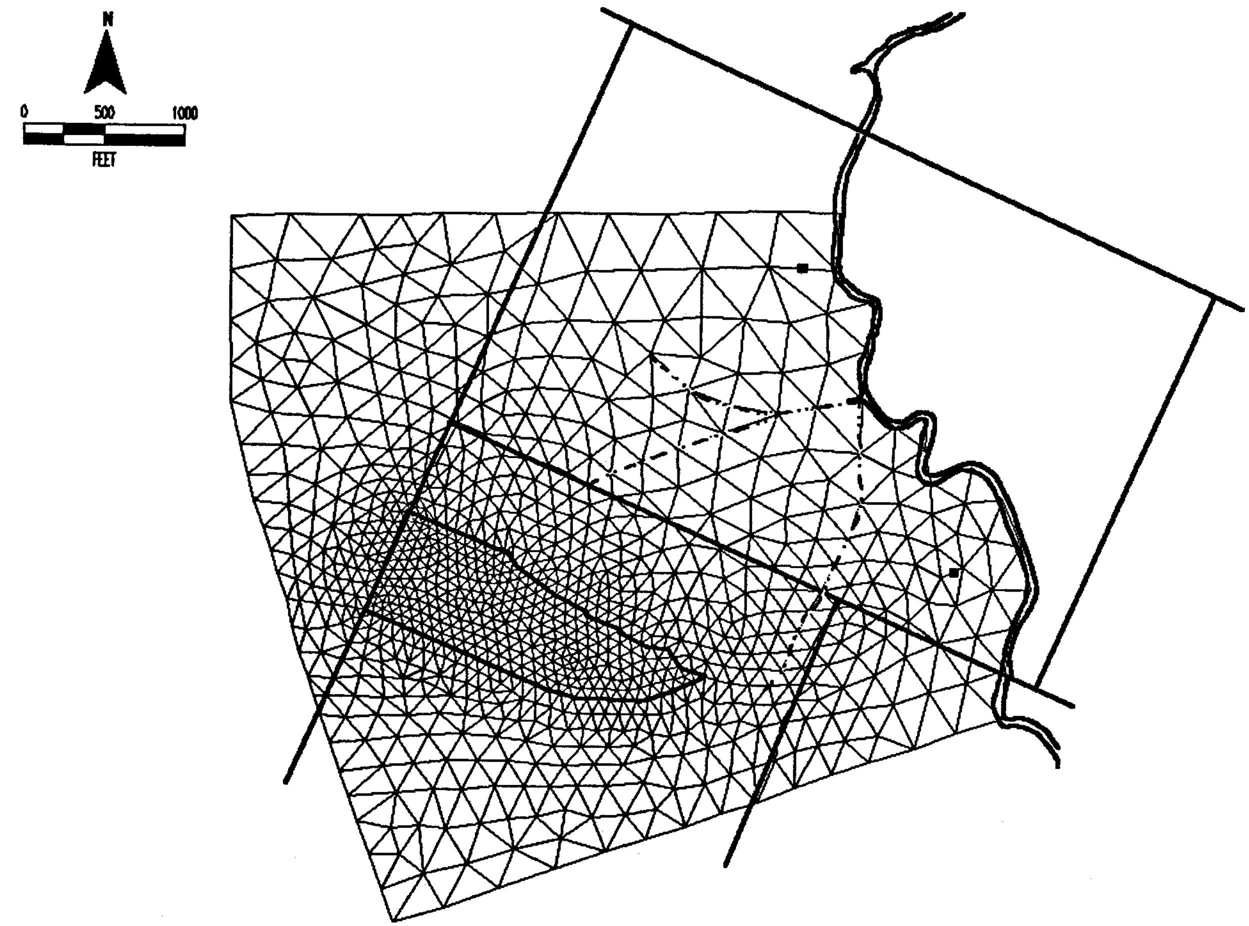
The finite element grid used in this analysis is shown superimposed on the base map of the TP Site in **Figure F-3**. The grid was developed such that all significant features, such as Chattanooga Creek and the Northwest and Northeast Tributaries, could be adequately represented in the model. The eastern side of the grid extends along Chattanooga Creek. None of the other sides of the grid extend along any surface water features, but are located far enough from the TP Site source areas such that all significant features affecting groundwater flow to and from the source areas are included in the model. The model grid consists of 869 nodes and 1673 elements.

The vertical grid consists of four levels of nodes that define three layers and two hydrostratigraphic units. One hydrostratigraphic unit (the bedrock zone) is divided into two layers for better discritization, particularly for the pumping scenarios described in Section F.3. The four node levels represent the following boundaries:

- Level 1 - Bottom of the aquifer (assumed to be 125 feet below the bedrock/soil overburden interface).
- Level 2 - 25 feet below the bedrock/soil overburden interface
- Level 3 - Bedrock/soil overburden interface
- Level 4 - Land surface

Cross-sectional views of the flow model hydrostratigraphic units are shown in **Figures F-4** and **F-5**. The size of the model area was selected based on the prevailing boundary conditions. DYNFLOW can simulate two types of boundary conditions. One is a specified head condition, and the other is a specified flow condition. With specified head conditions, the head is held constant at a predetermined elevation during the simulation. With specified flow conditions, the head may change, but the head gradient remains constant during the simulation. Ideally, model boundaries are chosen to coincide with actual stable hydrologic boundaries. Since Chattanooga Creek is the only true stable hydrologic boundary for the unconfined aquifer at the TP Site, the remaining model boundaries are located far enough from the source areas so that any realistic



MODEL FINITE ELEMENT GRID

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

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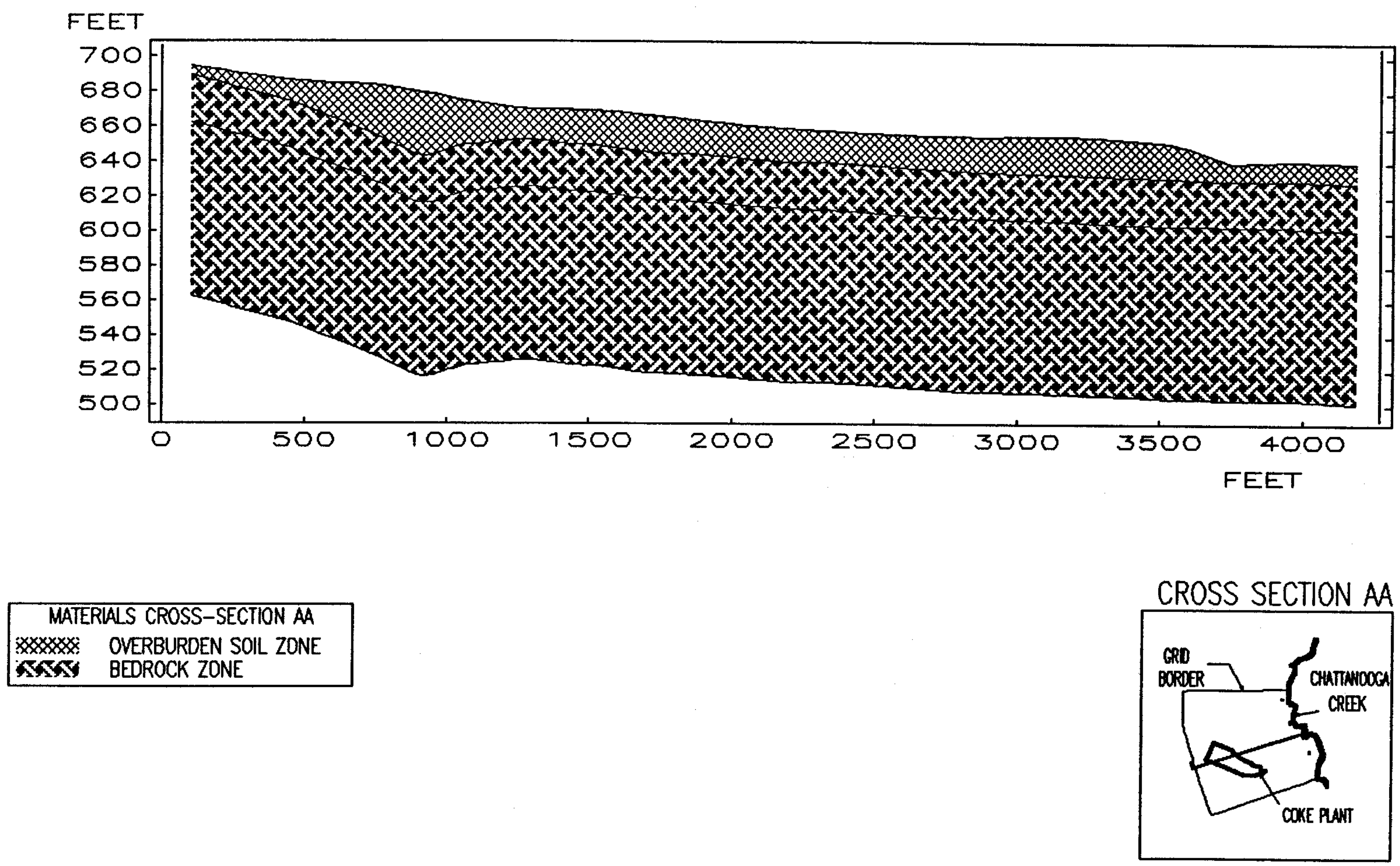

WEST-EAST MODEL HYDROSTRATIGRAPHIC CROSS SECTION

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

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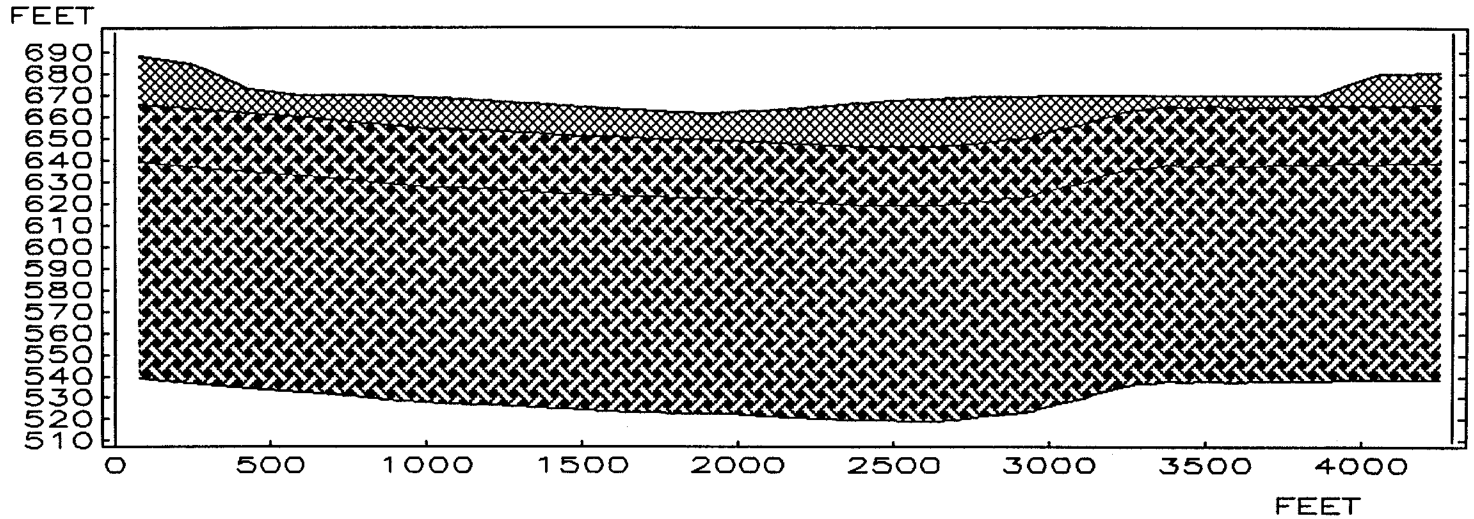
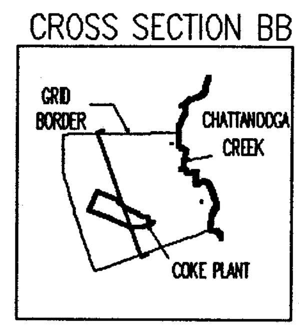


MATERIALS CROSS-SECTION BB
OVERBURDEN SOIL ZONE
BEDROCK ZONE



NORTH-SOUTH MODEL HYDROSTRATIGRAPHIC CROSS SECTION

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

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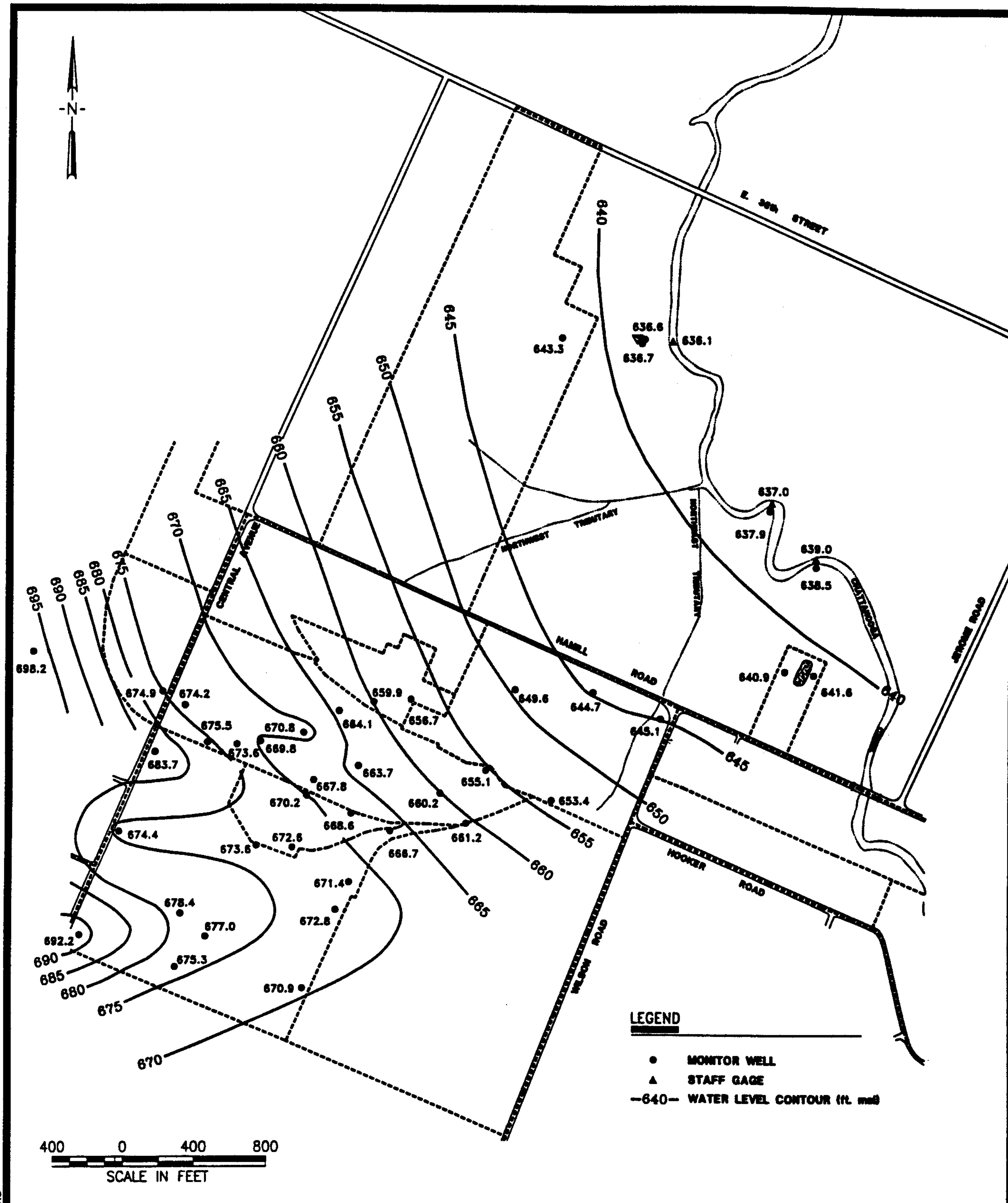
conditions imposed on these boundaries do not significantly alter simulation results at or near the source areas.

Boundary conditions imposed along the borders of the model vary between a specified head condition and a "no flow" condition, whichever is more representative of observed groundwater flow conditions in the aquifer. Based on the groundwater level contour map developed for the site during this remedial investigation (see **Figure F-6**), it appears that natural groundwater flow in the aquifer is toward the east. Specified head conditions were thus imposed along the eastern, western, and part of the southern borders of the grid while "no flow" conditions were imposed along the northern and rest of the southern borders as shown in **Figure F-7**. The distribution of specified heads along the eastern and western borders of the grid was estimated based on both the surface water and groundwater level measurements collected during this remedial investigation. At the bottom of the model (Level 1), a vertical "no flow" condition is also specified at evry node, thus preventing and vertical flow in or out of the model through the bottom of the aquifer. Streams and springs located in the interior of the model grid are represented through a "rising" head boundary condition. In these areas, the water table is allowed to rise to land surface, but not above it. If the water table is driven above the land surface, a discharge flux sufficient to keep the water table at land surface is introduced. This discharge flux represents the discharge of water that is lost from the groundwater system as surface water flow.

Two forms of aquifer stress are incorporated in the model: rainfall recharge and aquifer pumpage. No studies have been performed at the TP Site to determine rainfall recharge, and thus this parameter was included among the list of calibration parameters (see below). A study performed by Aller et al. (1987), however, indicates that rainfall recharge in the Nonglaciated Central Region, which includes the TP Site, may range from 0.2 to 20 inches per year. Presently, there is no significant pumping from the aquifer at the TP Site. However, the potential groundwater extraction alternatives evaluated with the model do include pumping. These remedial alternatives are discussed in Section F.3.



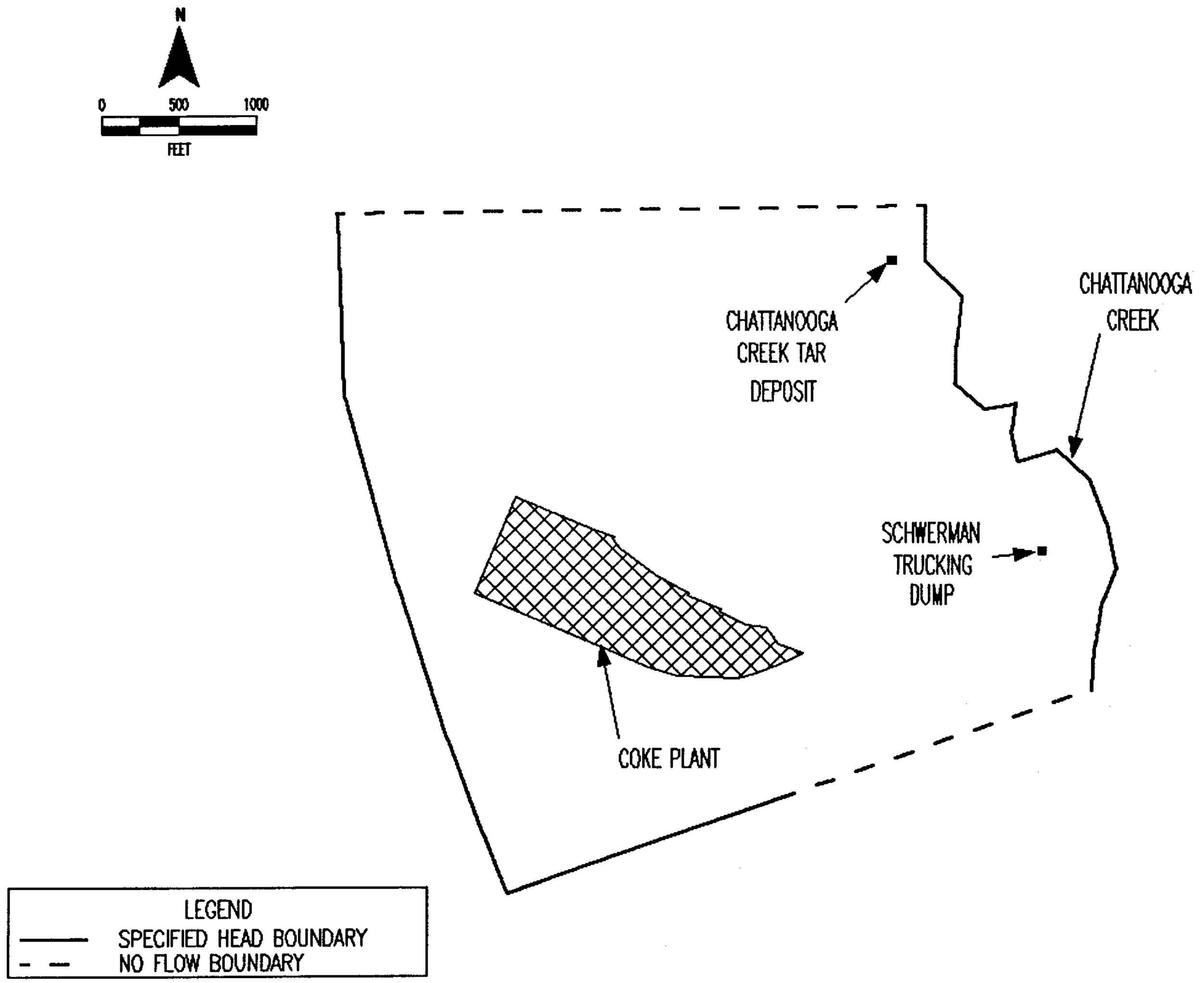
GW_JUN96/14JUN96/800

OBSERVED GROUNDWATER LEVELS - JUNE 1996

CDM FEDERAL PROGRAMS CORPORATION
a subsidiary of Camp Dresser & McKee Inc.

Tennessee Products Site
Chattanooga, Tennessee

FIGURE No. ~~2-5~~ F-6



MODEL BOUNDARY CONDITIONS

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

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F.1.3 FLOW MODEL CALIBRATION

Before a model can be used as a predictive tool, it should be calibrated to confirm that the model adequately represents groundwater flow in the aquifer system. The procedure for this involves selecting an inventory period from the past where data are sufficient to investigate the distribution of model parameters. Model-generated water levels, flows, and/or flow patterns are compared to observed water levels, flows, and/or flow patterns, and a sequence of adjustments in model parameters is made so that the predictions more closely reproduce the observations. During this process, however, the value of individual parameters must be kept within realistic limits. Parameters that are considered to be least reliable are usually modified more than other parameters.

The primary concern in the calibration process is the global response of the model. Although small areas within the model may not match historical data for all hydrologic conditions, systematic errors are investigated and eliminated, if possible, and focus is placed on the specific areas of interest. Differences between observed and computed water levels or flows do not necessarily invalidate the overall analysis. The scale of the model must be considered as well as the reliability and quantity of data. Water level and flow measurements are point measurements, which may be impacted by local stresses or heterogeneities, and thus may not be incorporated in the model due to their unknown existence and/or the lack of model resolution. The goal of the flow model, however, is not to simulate every local stress and heterogeneity if it is not within the resolution of the model, but to simulate general water levels, flows, and flow patterns for the scale and domain of the model.

The flow model for the TP Site was calibrated using water level measurements collected from monitor wells in the area during this remedial investigation (June 1996). These water level measurements are assumed to reflect steady-state or near steady-state conditions. The flow model developed in this study was thus calibrated under steady-state conditions. Steady-state conditions exist when flow into the aquifer system equals flow out of the aquifer system, and storage does not change with time. When calibrating under steady-state conditions, all aquifer parameters affect the results to some degree, except the storage coefficients (specific storativity and specific yield). The storage coefficients are only important when running the model in a transient (heads changing through time) mode. Therefore, the storage coefficients are not included in the calibrated flow model. In this study, all the scenarios were analyzed under steady-state conditions. Due to the slow movement of the contaminants in groundwater, short-term increases or decreases of water levels are not considered important. Therefore, storage coefficient estimates are not needed.

Prior to calibration, ranges of values for the various calibration parameters (horizontal and vertical hydraulic conductivities for the two hydrostratigraphic units, and rainfall recharge) were established and are presented in **Table F-1**. The ranges for the hydraulic conductivities are based on the data collected during this remedial investigation, other hydrogeologic investigations conducted in the area, as well as typical values determined for similar geologic materials. The range for rainfall recharge is based on the study performed by Aller et al. (1987). Note that the soil overburden hydrostratigraphic unit was divided into the following three zones: floodplain sediments, lowland soil, and upland soil. This zonal discretization for the same hydrostratigraphic unit is based on the observed hydraulic gradients across the site, as well as the results of hydraulic conductivity tests conducted at and around the site, both of which indicate distinct (order of magnitude) differences in hydraulic conductivity between the three zones. The model boundaries between each of these three zones are depicted in **Figure F-8**. Following each calibration run, the model-generated water levels and flow patterns were compared to the observed water levels and flow patterns, both visually and statistically, to help evaluate the effect of a given set of the input parameters (hydraulic conductivities and rainfall recharge) on the modeled water levels. In addition, a parameter optimization program was used to help guide the calibration process. The parameter optimization program used numerical optimization techniques to solve for the most likely distribution of hydraulic conductivities given the model structure and observed water levels. Over 30 calibration runs were made during the calibration process. The locations of the observation wells used for calibration (hereafter called calibration

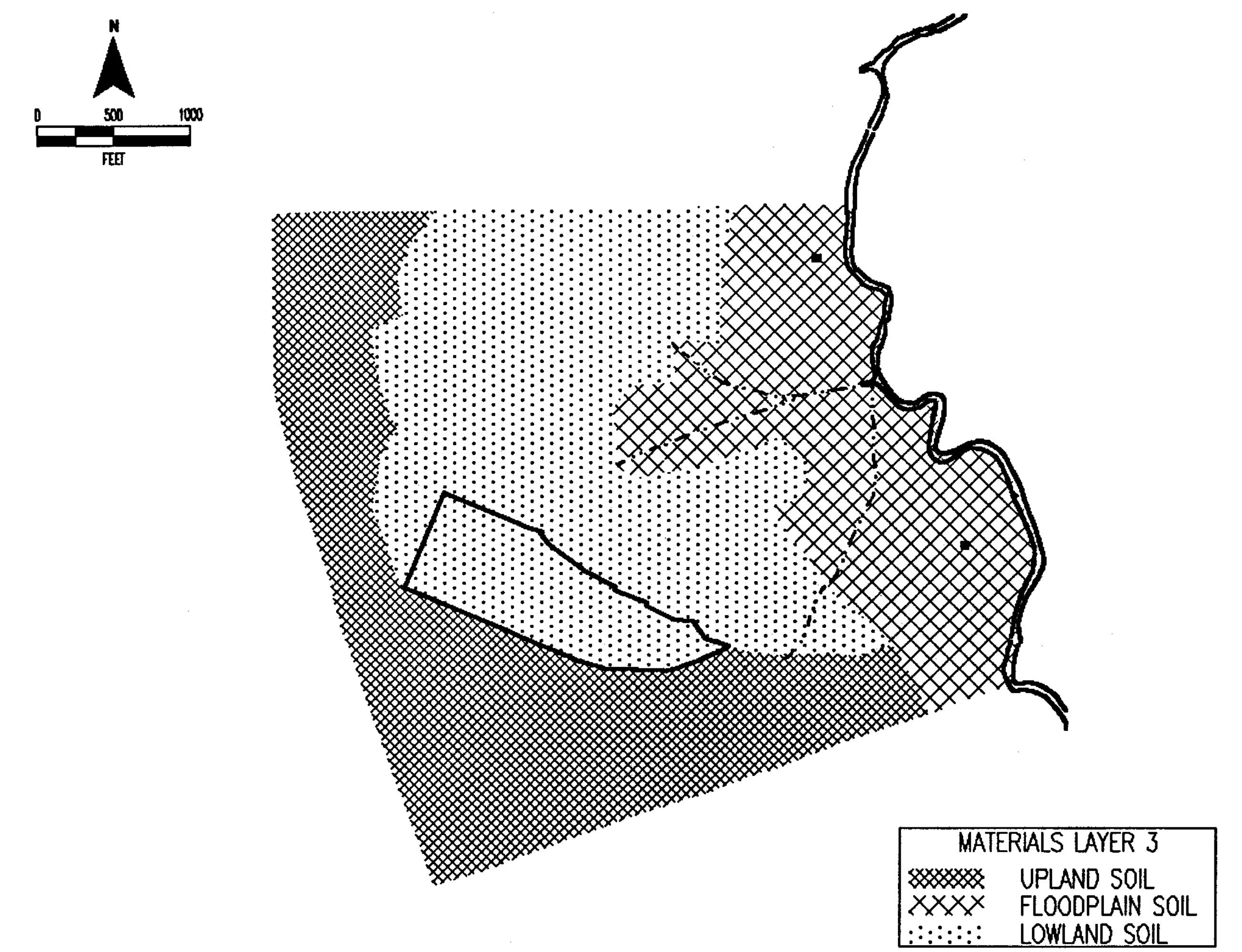
TABLE F-1

CALIBRATION PARAMETER RANGES
TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

Hydrostratigraphic Unit	Horizontal Hydraulic Conductivity (ft/day)		Horizontal:Vertical Hydraulic Conductivity Ratio		Rainfall Recharge (inches/year)	
	Low	High	Low	High	Low	High
Soil Overburden						
Upland Zone	0.1	1	1:1	100:1	0.2	20
Lowland Zone	1	30	1:1	100:1	0.2	20
Floodplain Zone	30	300	1:1	100:1	0.2	20
Bedrock	0.1	10	1:1	100:1	NA	NA

Note:

NA - Not Applicable



SOIL OVERBURDEN ZONES

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

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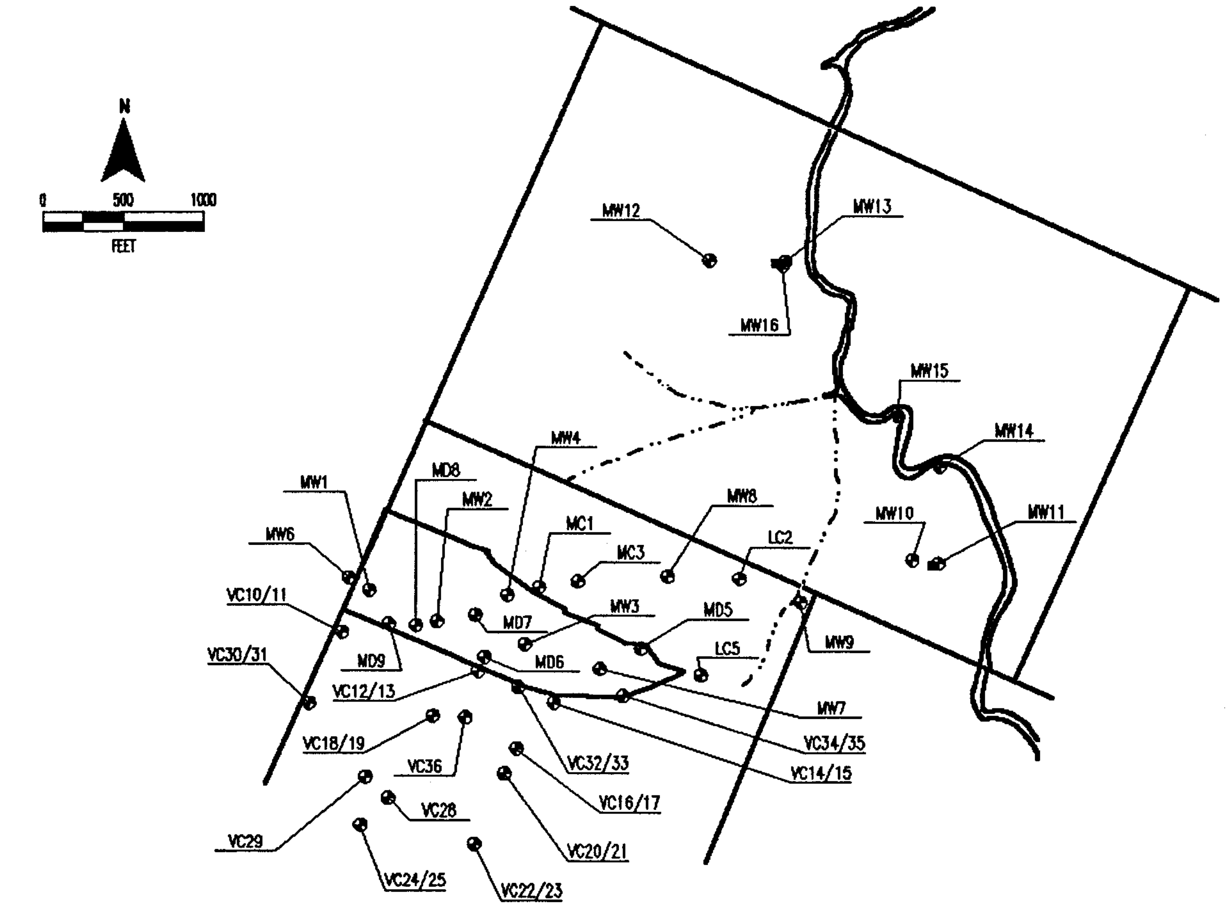
wells) are shown in **Figure F-9**. The final calibration parameter values are presented in **Table F-2**. A comparison of the simulated water levels and the observed water levels is presented in **Table F-3**, and the spatial variations of the differences between simulated and observed water levels in the soil overburden monitor wells and the bedrock monitor wells are shown in **Figures F-10** and **F-11**, respectively. A summary of the statistics for the model calibration results is presented in **Table F-4**. The simulated water level contour map is shown in **Figure F-12**. As seen in the above figures and tables, model results compare quite favorably to the observed data. Simulated flow patterns are very similar to observed flow patterns and, with a head variation of approximately 62 feet across the site, a standard deviation of differences of 1.90 is considered to be very good. A few wells show large differences between observed and simulated water levels, the greatest being 5.5 feet, but these differences are probably due to local heterogeneities in the aquifer system. Due to their unknown characteristics or to the limited model resolution, these local hetrogeneities could not be incorporated in the model. These differences, although important on a local scale, are not as significant with regard to the scale of the model, and therefore do not invalidate the results of this study.

F.2 CONTAMINANT TRANSPORT MODEL DEVELOPMENT

The next step in this study was to develop a compatible contaminant transport model to simulate the potential movement of the contaminants of concern in the aquifer system. These models can vary from simple analytical equations to complex numerical computer models. Because of the complexity of this contaminant transport problem, the companion contaminant transport model for DYNFLOW called DYNTRACK (DYNamic particle TRACKing) was selected.

DYNTRACK is a computer program that simulates three-dimensional contaminant transport in the saturated zone of an aquifer system, and uses the same three-dimensional finite element grid discretization used for DYNFLOW. DYNTRACK can simulate contaminant movement for conservative constituents with dispersion, as well as constituents subject to first-order decay



CALIBRATION WELL LOCATIONS

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

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TABLE F-2

FINAL CALIBRATION PARAMETER VALUES
TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

Hydrostratigraphic Unit	Horizontal Hydraulic Conductivity (ft/day)	Vertical Hydraulic Conductivity (ft/day)	Rainfall Recharge (inches/year)
Soil Overburden			
Upland Zone	0.4	0.1	6
Lowland Zone	12	0.12	6
Floodplain Zone	62	31	6
Bedrock	0.7	0.03	NA

Note:

NA - Not Applicable

TABLE F-3

CALIBRATION WELL OBSERVED AND SIMULATED WATER LEVELS
TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

Unit	Well ID	Observed Head (ft msl)	Simulated Head (ft msl)	Difference (ft)
Soil Overburden	MW1-SH	673.69	672.91	0.78
	MW2-SH	669.98	670.00	-0.02
	MW3-SH	665.23	663.82	1.41
	MW4-SH	664.79	664.36	0.43
	MW6-SH	674.66	672.98	1.68
	MW7-SH	660.78	660.22	0.56
	MW8-SH	652.65	649.55	3.10
	MW9-SH	643.31	645.38	-2.07
	MW10-SH	640.38	641.20	-0.82
	MW11-SH	640.01	642.09	-2.08
	MW12-SH	642.02	644.36	-2.34
	MW13-SH	637.73	636.59	1.14
	MW14-SH	638.49	638.49	0.00
	MW15-SH	637.84	637.93	-0.09
	MW16-SH	637.94	636.68	1.26
	MD5-12	657.54	654.42	3.12
	MD6-14	667.56	667.04	0.52
	MD7-12	667.58	671.06	-3.48
	MD9-20	672.51	675.50	-2.99
	MC1	662.24	659.87	2.37
	MC3	659.21	656.72	2.49
	LC2	646.84	644.68	2.16
	LC5	653.75	653.36	0.39
	VC10	678.80	684.30	-5.50
	VC12	668.43	670.85	-2.42
	VC14	665.80	666.38	-0.58
	VC16	670.77	671.38	-0.61
	VC20	671.58	672.76	-1.18
	VC22	671.18	671.26	-0.08
	VC24	677.79	674.81	2.98
	VC28	677.78	677.03	0.75

TABLE F-3 (cont.)

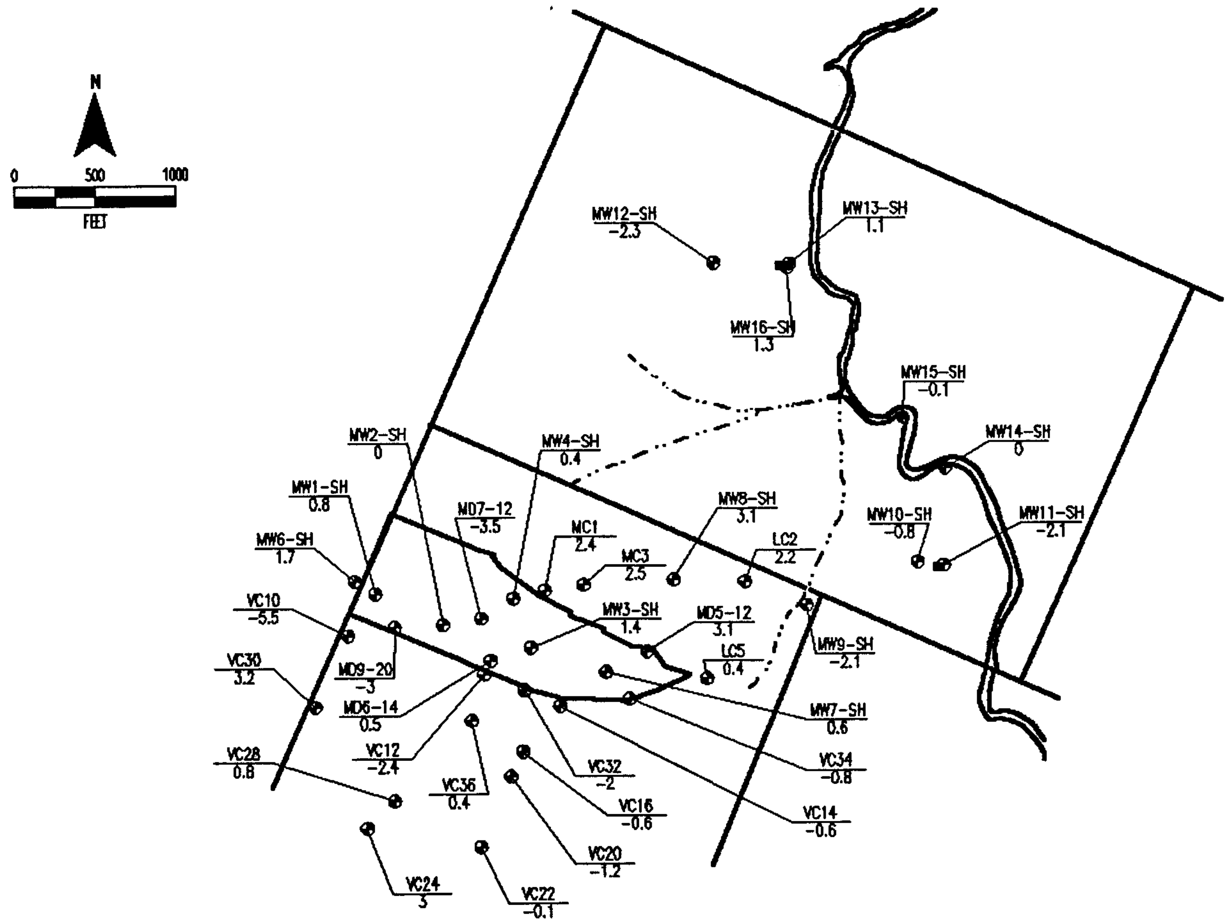
**CALIBRATION WELL OBSERVED AND SIMULATED WATER LEVELS
TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE**

Unit	Well ID	Observed Head (ft msl)	Simulated Head (ft msl)	Difference (ft)
Soil	VC30	677.28	674.08	3.20
Overburden	VC32	666.80	668.84	-2.04
(cont.)	VC34	660.32	661.14	-0.82
	VC36	672.91	672.55	0.36
Bedrock	MW1-DP	675.14	675.27	-0.13
	MW2-DP	670.24	670.63	-0.37
	MW3-DP	664.93	662.24	2.69
	MW4-DP	664.55	662.18	2.37
	MW1-IN	674.07	675.41	-1.34
	MW2-IN	669.99	669.60	0.39
	MW3-IN	665.10	663.56	1.54
	MW4-IN	664.60	663.85	0.75
	MW6-IN	675.31	676.80	-1.49
	MW7-IN	660.66	660.25	0.41
	MW8-IN	652.71	649.60	3.11
	MW9-IN	643.30	644.86	-1.56
	MW10-IN	640.42	640.58	-0.16
	MW11-IN	640.04	641.10	-1.06
	MW12-IN	642.17	642.17	-0.00
	MD5-20	657.45	655.78	1.67
	MD6-73	668.05	668.56	-0.51
	MD7-51	667.45	670.55	-3.10
	MD8-63	671.70	673.55	-1.85
	VC11	678.62	683.17	-4.55
	VC13	668.71	669.65	-0.94
	VC15	665.63	667.03	-1.40
	VC19	673.97	673.65	0.32
	VC21	670.70	672.81	-2.11
	VC23	670.40	670.52	-0.12
	VC25	677.17	675.70	1.47

TABLE F-3 (cont.)

**CALIBRATION WELL OBSERVED AND SIMULATED WATER LEVELS
TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE**

Unit	Well ID	Observed Head (ft msl)	Simulated Head (ft msl)	Difference (ft)
Bedrock	VC29	678.08	678.41	-0.33
(cont.)	VC31	676.72	674.63	2.09
	VC33	666.91	668.38	-1.47
	VC35	660.75	661.34	-0.59



SIMULATED vs. OBSERVED WATER LEVEL DIFFERENCES
IN SOIL OVERBURDEN MONITOR WELLS
TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

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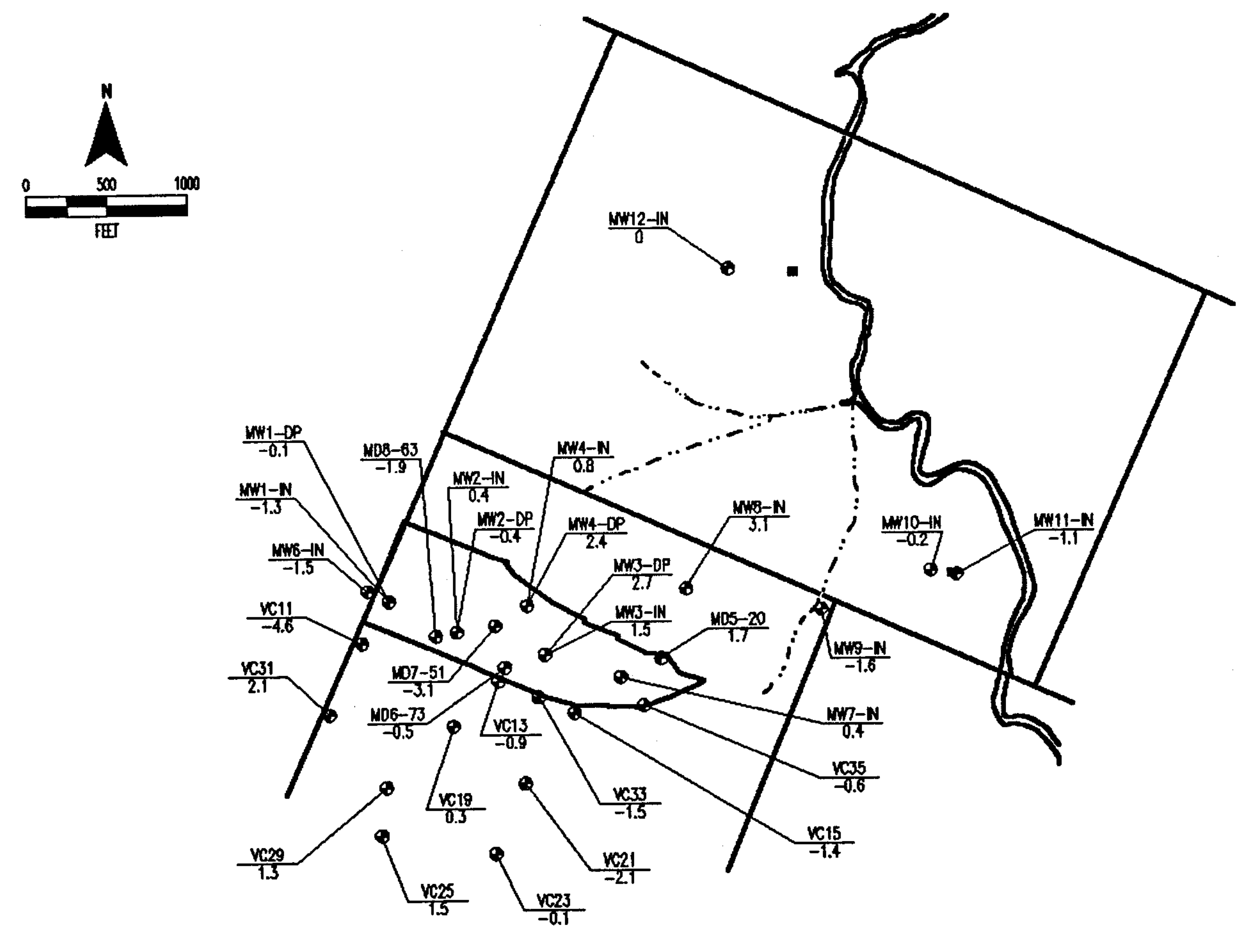

SIMULATED vs. OBSERVED WATER LEVEL DIFFERENCES
IN BEDROCK MONITOR WELLS
TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

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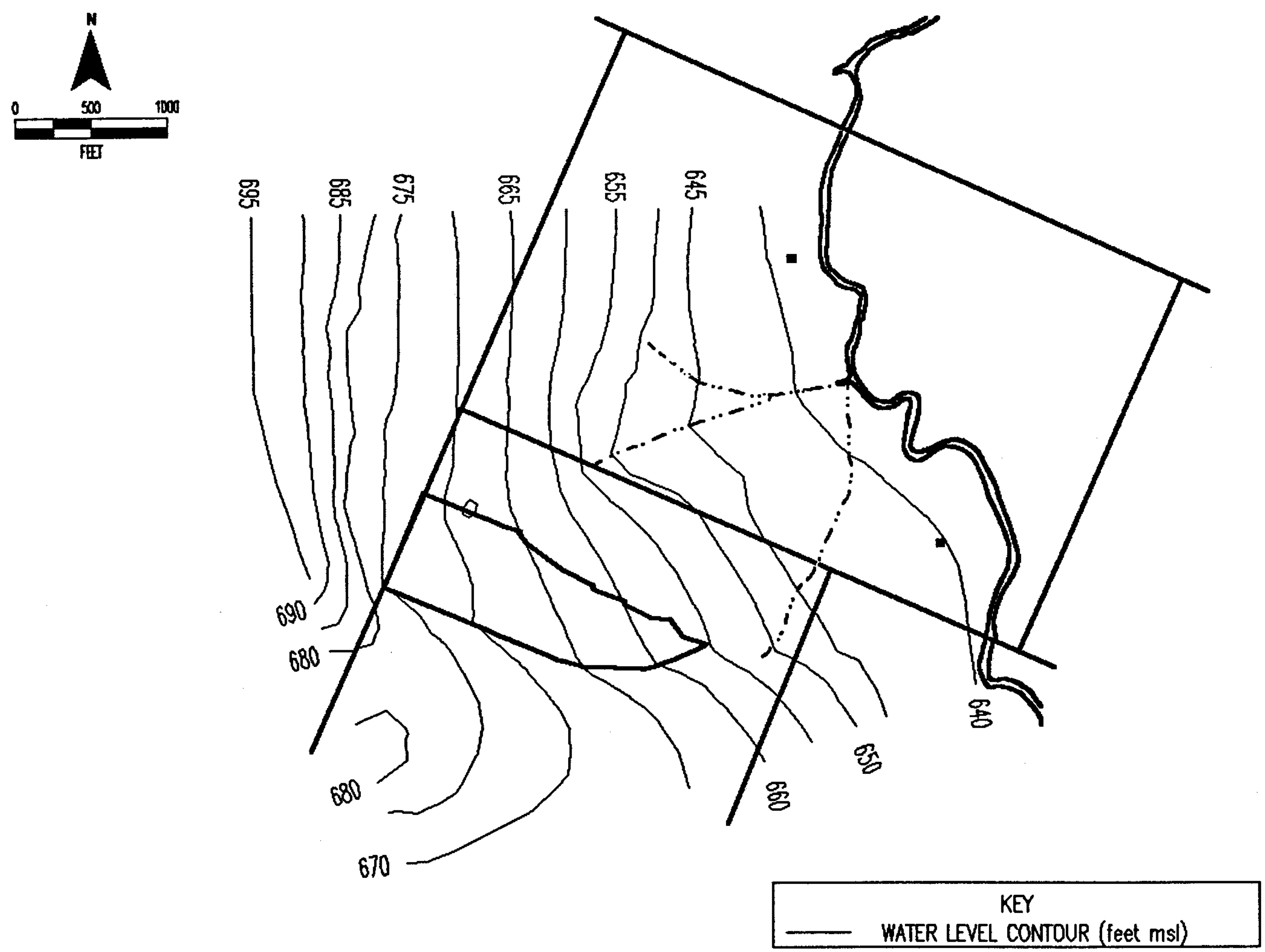
TABLE F-4

CALIBRATION SUMMARY STATISTICS
TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

Unit	Average Water Level Difference (feet)	Standard Deviation of Differences (feet)
Soil Overburden	0.05	2.06
Bedrock	-0.15	1.74
Overall	-0.07	1.90



SIMULATED GROUNDWATER LEVELS – PRESENT CONDITIONS

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

F–12

and/or adsorption. Thus, DYNTRACK permits the evaluation of complicated contaminant transport problems.

F.2.1 MODEL DESCRIPTION

Two basic approaches historically have been taken in the analysis of contaminant movement: the Eulerian and the Lagrangian. The Eulerian approach solves the governing mass transport equation directly, generally using finite element or finite difference techniques, and provides a continuous contaminant field. This approach analyzes the variation over time of a variable (in most cases, contaminant concentration) at fixed points within the region.

The Lagrangian approach analyzes the variation in time and space of a fixed value (mass of contaminant). This method is usually implemented using a random walk technique for a statistically significant numbers of particles (each of which represents a discrete parcel of mass). DYNTRACK uses this approach.

Random Walk Method

The differential equation describing transport of conservative contaminants in groundwater flow is as follows:

$$\theta \frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij} \frac{\partial C}{\partial x_j}\right) - q_i \frac{\partial C}{\partial x_i}$$

where,

C	=	concentration (mass/length^3)
θ	=	effective porosity
q_i	=	specific discharge (length/time)
D_{ij}	=	dispersion coefficient matrix (length^2/time)

$t \quad = \quad$ time

Note that the first item on the right-hand side of the equation represents the dispersive flux as embodied by Fick's Law, and the second represents the convective flux.

As noted previously, DYNTRACK uses the random walk method to solve this contaminant transport equation. This method utilizes a statistical model of the microscopic movement of pollutant "particles". Each particle has an associated weight, decay rate, and retardation rate. Contaminant concentration is computed from the particle distribution at any time as the total particle weight divided by the water volume in which the specific particles reside. The model operates by moving particles within a computed hydraulic gradient field (DYNFLOW) in discrete time steps. Velocities computed from the simulated head field are used to compute the convective movement of the particles during a given time step. A random component is then added to simulate the effect of dispersion. In DYNTRACK, a random deflection based on a given probability density function is directly related to the dispersion coefficient. Total contaminant mass within a given groundwater volume provides a measure of the contaminant concentration. Thus, as the total number of particles representing a given mass is increased, the approximation becomes more accurate.

The application of the random walk method as used by DYNTRACK is documented in the DYNTRACK Users Manual (CDM, 1984b). In addition, several excellent descriptions of the fundamentals behind this method exist in the literature (Bear, 1972; Fischer, et al., 1979; Weiss, 1983).

Data Requirements

As noted previously, DYNTRACK uses the same three-dimensional finite element grid representation of aquifer geometry, flow field, and hydrostratigraphy as in DYNFLOW. Additional data requirements include specification of values for the following properties:

- Effective Porosity - connected or mobile pore space
- Longitudinal Dispersivity - coefficient used to calculate dispersion in the direction of mean flow
- Transverse Dispersivity - coefficient used to calculate dispersion in the direction perpendicular to mean flow
- Vertical Dispersion Anisotropy Factor - coefficient used to calculate the suppression of vertical dispersion due to the bedded nature of geologic units
- Contaminant Decay Rate - coefficient used to calculate first order decay of a contaminant
- Retardation Factor - Coefficient used to calculate sorption of contaminants

Other data requirements include the specification of the contaminant source loading rates and locations.

F.2.2 MODEL SETUP

Because of the lack of reliable and well-defined contaminant source data at the TP Site, calibration of the contaminant transport properties described above was not possible. Instead, best estimates of the contaminant transport properties were used in the model. Best estimates of the first five contaminant transport properties described above are presented in **Table F-5**. These estimates are based values sited by Walton (1984) for similar geologic units as are present at the TP Site, as well as previous modeling studies performed by CDM Federal for similar sites. Note that to be conservative, all contaminant decay rates were set equal to zero, even though biodegradation may in reality cause some of the contaminants of concern to decay in the aquifer system. Best estimates of the retardation coefficients for the contaminants of concern are presented in **Table F-6**.

TABLE F-5

BEST ESTIMATES OF CONTAMINANT TRANSPORT PROPERTIES
TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

Parameter	Soil Overburden	Bedrock
Effective Porosity (dimensionless)	0.2	0.05
Longitudinal Dispersivity (feet)	50	50
Transverse Dispersivity	10	10
Vertical Dispersion Anisotropy Factor	0.1	0.1
Contaminant Decay Rate	0*	0*

Note:

* - Conservative Estimate

TABLE F-6

BEST ESTIMATES OF RETARDATION COEFFICIENTS
TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

Contaminant of Concern	Soil/Water Partition Coefficient (ml/g)	Retardation Coefficient
Inorganics		
Arsenic	200[1]	1500
Aluminum	1[2]	8.7
Barium	0.5[1]	4.8
Beryllium	1300[1]	10000
Cadmium	560[1]	4300
Iron	170[1]	1300
Manganese	180[1]	1400
Nickel	650[1]	5000
Vanadium	10[2]	78
Cyanide	0.1[2]	1.8
VOCs		
Acetone	0.00045[1]	1.0
Benzene	0.11[1]	1.8
Carbon Tetrachloride	0.33[1]	3.5
Chlorobenzene	0.52[1]	5.0
Chloroform	0.070[1]	1.5
1,2-Dichloroethane	0.023[1]	1.2
Ethylbenzene	1.1[1]	9.5
Methyl Butyl Ketone	0.018[1]	1.1
Tetrachloroethene	0.57[1]	5.4
Toluene	0.37[1]	3.8
1,1,1-Trichloroethane	0.11[1]	1.8
Trichloroethene	0.15[1]	2.2

TABLE F-6 (cont.)

BEST ESTIMATES OF RETARDATION COEFFICIENTS
TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

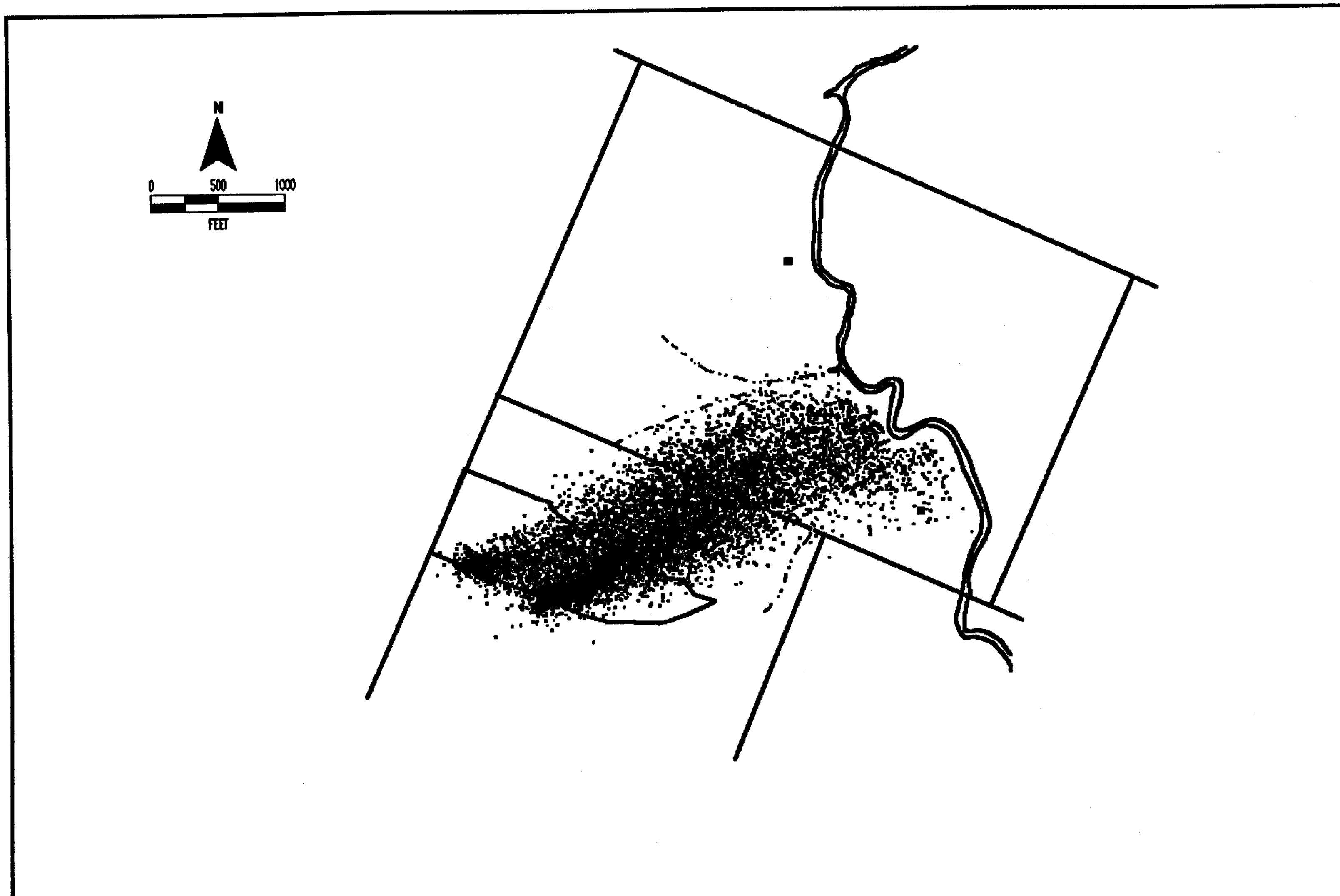
Contaminant of Concern	Soil/Water Partition Coefficient (ml/g)	Retardation Coefficient
SVOCs		
Benzo(a)anthracene	110[1]	850
Benzo(b &/or k)fluoranthene	2800[1]	22000
Benzo-a-pyrene	830[1]	6400
Bis(2-ethylhexyl)phthalate	410000[1]	3200000
Carbazole	3.9[1]	31
Dibenzo(a,h)anthracene	700[1]	5400
Dibenzofuran	11[1]	86
1,4-Dichlorobenzene	1.8[1]	15
2,4-Dimethylphenol	0.24[1]	2.8
Indeno(1,2,3-cd)pyrene	35000[1]	270000
2-Methylnaphthalene	9.8[1]	76
2-Methylphenol	0.067[1]	1.5
(3-and/or 4-)Methylphenol	0.063[1]	1.5
Naphthalene	1.7[1]	14
Phenanthrene	22[1]	170
Pesticides/PCBs		
Alpha-BHC	4.9[1]	39
Beta-BHC	4.8[1]	37
Delta-BHC	11[1]	86
Dieldrin	110[1]	850
PCB-1248	420[1]	3200

NOTES:

1) See Table 8-2.
2) Conservative estimate - no data available

a particle tracking simulation to evaluate migration pathways and potential extent of contamination from the coke plant source area. Contaminant concentrations were not considered in this scenario.

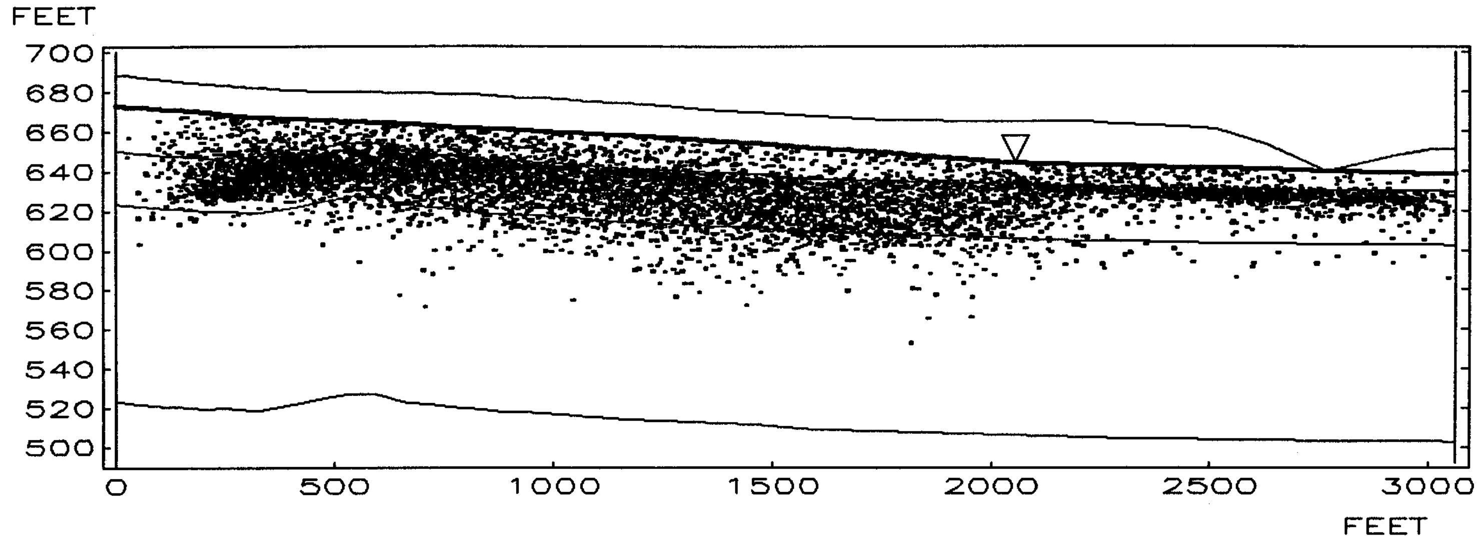
This scenario was divided into three parts. In the first part (Scenario #1A), the retardation coefficient was set equal to 1.0, thus representing those contaminants which do not significantly sorb to the soil matrix and thus generally move as groundwater moves (i.e., most of the VOCs, the phenols, barium, and possibly cyanide). In the second part (Scenario #1B), the retardation coefficient was set equal to 10, thus representing those contaminants which are moderately sorbed to the soil matrix (i.e., ethylbenzene, the BHC pesticides, the lower molecular weight PAHs, dibenzofuran, 1,4-dichlorobenzene, and possibly aluminum and vanadium). In the third part (Scenario #1C), the retardation coefficient was set equal to 100, thus representing those contaminants which are greatly sorbed to the soil matrix (i.e., the higher molecular weight PAHs, phthalates, dieldrin, PCBs, and the rest of the metals). The simulation results for this scenario are shown in **Figures F-13** through **F-18**, where the particle plumes for each of the three parts are shown in plan view and cross-section view. The results indicate that the highly mobile contaminants (i.e., those with a retardation coefficient less than 10) could have moved a significant distance from their source in the 78 years since operations began at the coke plant facility, and may have even reached and discharged into Chattanooga Creek. In addition, some of the highly mobile contaminants could have discharged into the Northwest Tributary or the Northeast Tributary. Migration of the lesser mobile contaminants (i.e., those with a retardation coefficient greater than 10) in groundwater, however, has likely been limited primarily to the area south of Hamill Road, with some of the lesser mobile contaminants (i.e., those with a retardation coefficient greater than 100) not having moved any significant distance from the source areas, due to the high rate of sorption of these contaminants.



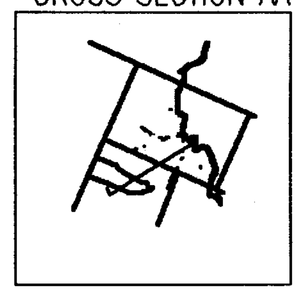
SIMULATED PARTICLE PLUME (PLAN VIEW) – SCENARIO #1A

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

F–13



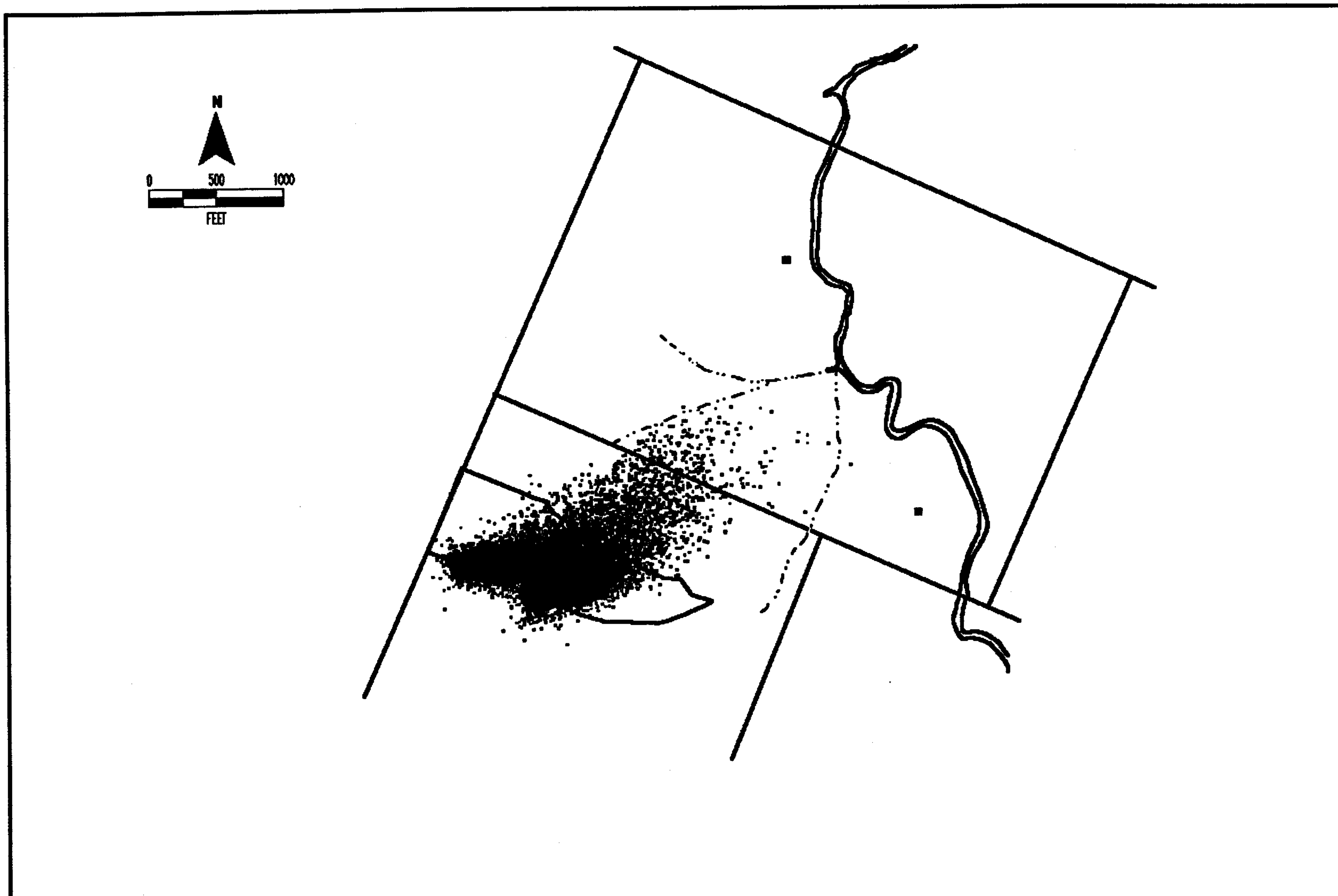
CROSS SECTION AA



SIMULATED PARTICLE PLUME (CROSS SECTION) - SCENARIO #1A

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

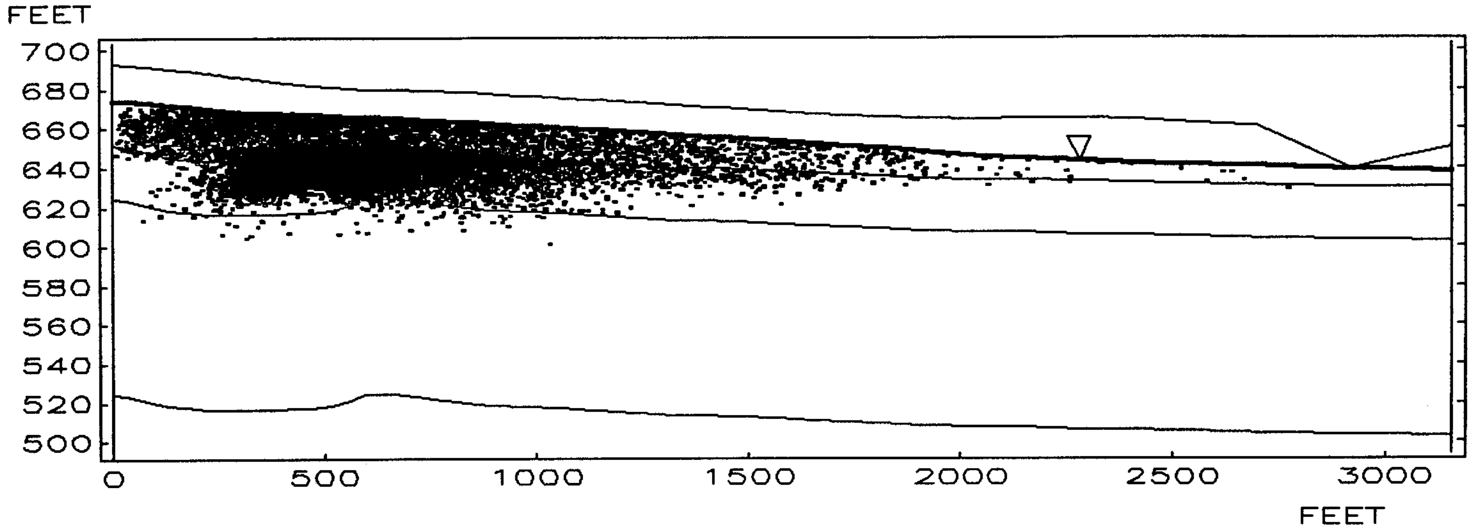
F-14



SIMULATED PARTICLE PLUME (PLAN VIEW) – SCENARIO #1B

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

F–15



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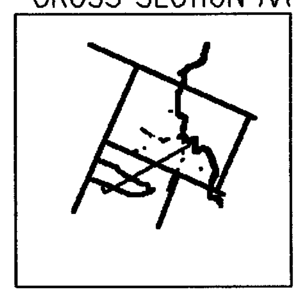
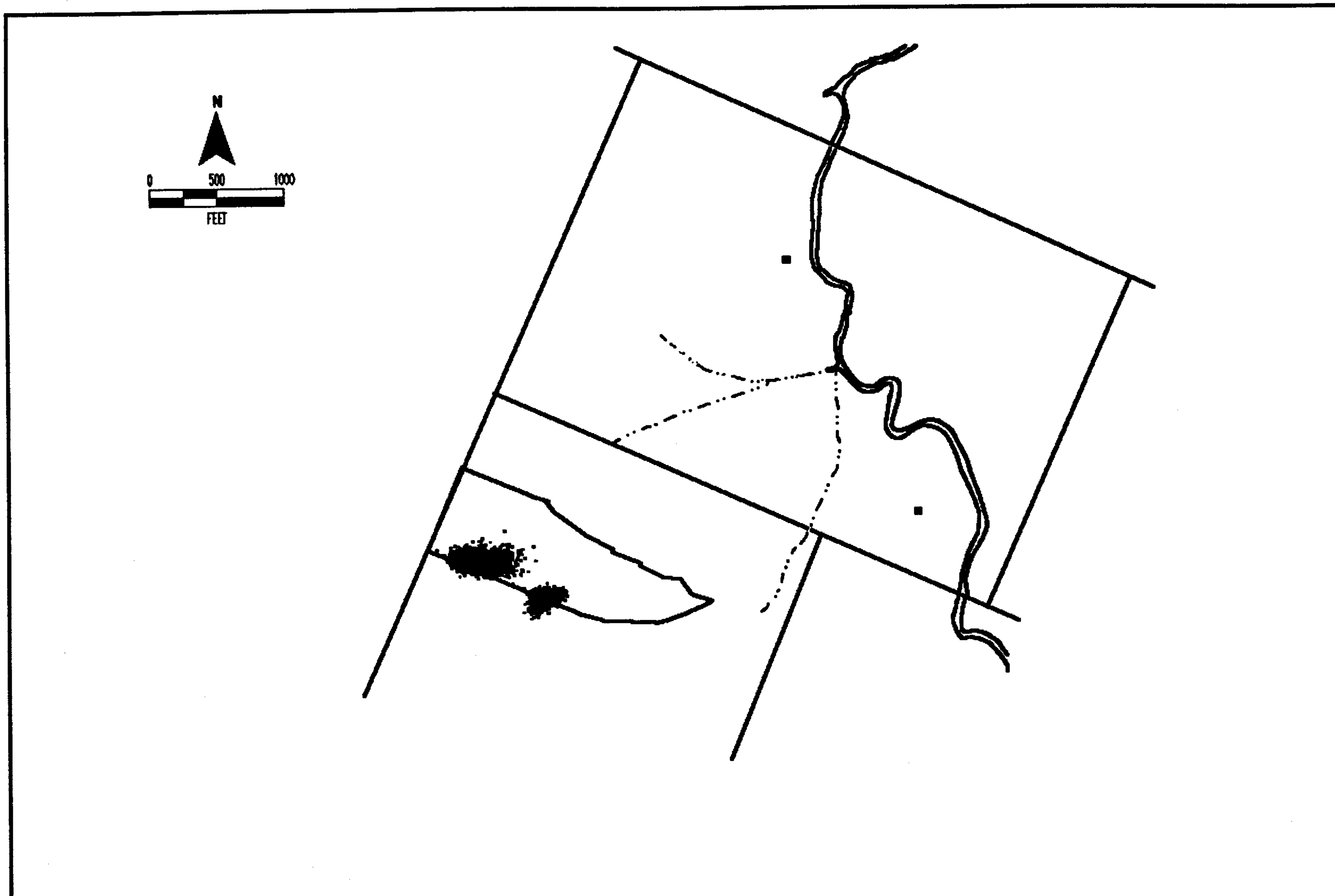


SIMULATED PARTICLE PLUME (CROSS SECTION) – SCENARIO #1B

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

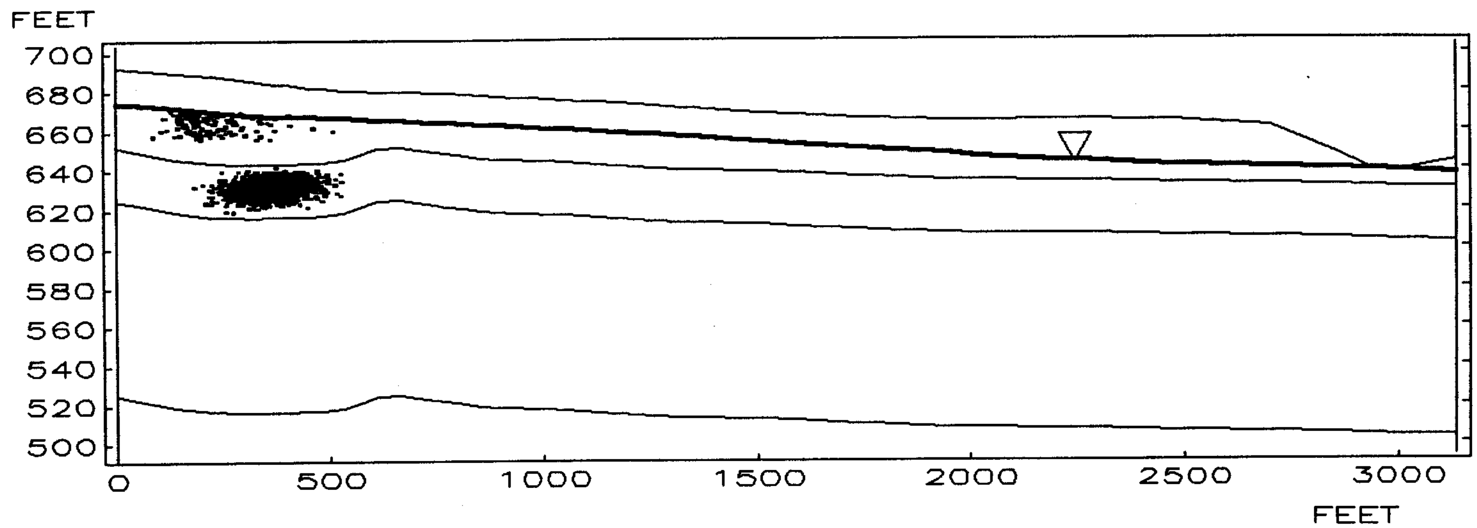
F-16



SIMULATED PARTICLE PLUME (PLAN VIEW) – SCENARIO #1C

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

F–17



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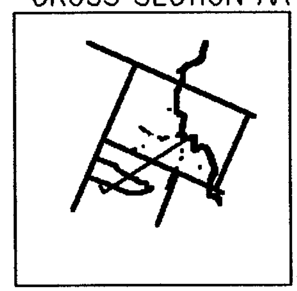

SIMULATED PARTICLE PLUME (CROSS SECTION) – SCENARIO #1C

TENNESSEE PRODUCTS SITE
CHATTANOOGA, TENNESSEE

F–18

REFERENCES

Aller, L., Bennett, T., Lehr, J.H., Petty, R.J., and Hackett, G., 1987. *DRASTIC: A Standardized System for Evaluating Ground Water Pollution Potential Using Hydrogeologic Settings*, prepared under a cooperative agreement between the National Water Well Association and the U.S. Environmental Protection Agency, EPA-600/2-87-035.

Bear, J., 1972. *Dynamics of Fluids in Porous Media*, American Elsevier, New York.

Camp Dresser & McKee Inc., 1984a. *DYNFLOW - A Three-Dimensional Finite Element Groundwater Flow Model, Description and User's Manual*, unpublished.

Camp Dresser & McKee Inc., 1984B. *DYNTRACK - A Three-Dimensional Contaminant Transport Model for Groundwater Studies, Description and User's Manual*, unpublished.

Fischer, H.B., List, E.J., Koh, R.C.Y., Imberger, J., and Brooks, N.H., 1979. *Mixing in Inland and Coastal Waters*, Academic Press.

Oak Ridge National Laboratory, 1991. *The Effectiveness of Groundwater Pumping as a Restoration Technology*, ORNL/TM-11866.

Pinder, G.F., and Gray, W.G., 1977. *Finite Element Simulation in Surface and Subsurface Hydrology*, Academic Press.

Weiss, G.H., 1983. *Random Walks and Their Applications*, American Scientist, January/February.

Wilson, J.L., Townley, L.R., and Sa Da Costa, A.G., 1979. *Mathematical Development and Verification of a Finite Element Aquifer Flow Model AQUIFEM-1*, Department of Civil Engineering, Massachusetts Institute of Technology, TAP Report 79-3, Cambridge, Massachusetts.